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Thermal effect on mobility of colour centers in alkali halide crystals

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Abstract : Electron injection has been carried out in single crystals of pure KCl and KBr under constant field for different temperatures. The injection current and optical density as a function of time are measured for both growth and decay process to estimate the mobility of colour center. The activation energy for bleaching of trapped centers and corresponding dissociation energy have been calculated.

Keywords : Alkali-halide, colour center.

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1. Introduction

It is well known that alkali halides are typical insulators with a forbidden band gap of 10 eV and they behave extraordinary wide range of optical transparency from far UV to far IR. The conduction band does not give rise to any conductivity since it contains no electrons and neither does the valence band conduct since there are no unoccupied states into which electron can be accelerated by the electric field. This simple picture applies only to a perfect crystalline insulator at absolute zero of temperature. The energy band diagram for the injection of electrons into the crystalline dielectrics through heterogeneous metal-insulator-metal contact [1,2] provides the basis for creating defect centers within the bulk. On completion of the ionic stage (zone-I) the conductivity of the crystalline insulator gradually increases with the formation of colour centers. On reversing the field, the electrons are de-trapped, thereby, decreasing the colour centers as well as the conductivity of the crystal. Here temperature plays an important parameter to execute the process. In the present paper the decay of colour centers has been studied and mobility of those trapped centers are evaluated (under different thermal stresses) yielding the activation energy for thermal dissociation of the trapped centers.

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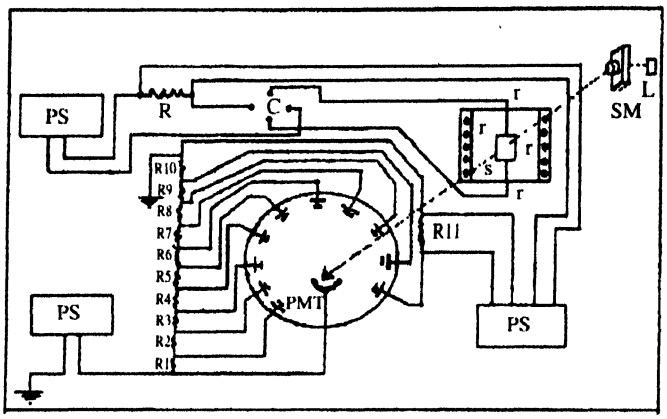
2. Experimental

Pure KCl and KBr single crystals are grown in the laboratory by the Czochralski-Kyropolous method, using a microprocessor controlled furnace under argon atmosphere and servo-controlled rotation pulling arrangement. Rotation rate of crucible is of the order of 5–8 rpm and pulling rate of seed is 120 μm min^{-1}. The temperature of the furnace is 1150 K for KCl growth and 1100 K for KBr growth. Figure 1 shows the grown crystals by Czochralski-Kyropolus method in our laboratory. The purity of the crystals has been tested with the help of Laue diffraction pattern (not shown).

Figure 1. Grown crystals by Czochralski-kyropolus method.

The typical experimental arrangement is shown in Figure 2. Crystals are cleaved along the <100> direction



I : Light Source, SM : Spectrometer, FF : Electrical Furnace, EF : electrodes, S : Specimen, C : Commutator, PS : Power Supply, PR : Pen-Recorder, PMT : Photo-Multiplier Tube.

Figure 2. General experimental arrangement.

and surface polished. A sample is placed between a heterogeneous contact of flat platinum anode and a sharp pointed brass cathode [2–6]. The system is housed in an electrical furnace for electron injection. The injection experiment has been carried out at constant fields of 710 V cm^{-1} under different temperatures ambient between 795 K to 945 K. The process is stopped well before the commencement of third zone [7]. The decay of colour centers is augmented by reversing the electric field and the process is continued till the crystal regains its original transparency. The pristine time has been checked. By shining the specimen with appropriate F-light using reflection grating monochromator (ORIEL, USA) the colour center or the transparency of crystals have been studied. The transmitted light through a crystal has been recorded by photo-multiplier detector system. Injection and photo current have been recorded simultaneously during growth and decay processes with the help of a Bausch and Lomb series 5000 strip chart two pen recorder.

3. Result and discussion

When the polarity of the electrode is reversed *i.e.* pointed electrode is positive and flat one is negative there is no question of creation of high electron density near cathode. In stead of being created, the F-centers will migrate towards high affinity side *i.e.* pointed electrode. The situation of such experimental fact may be analyzed in this way. The change of optical density during decay process has been shown in Figure 3.

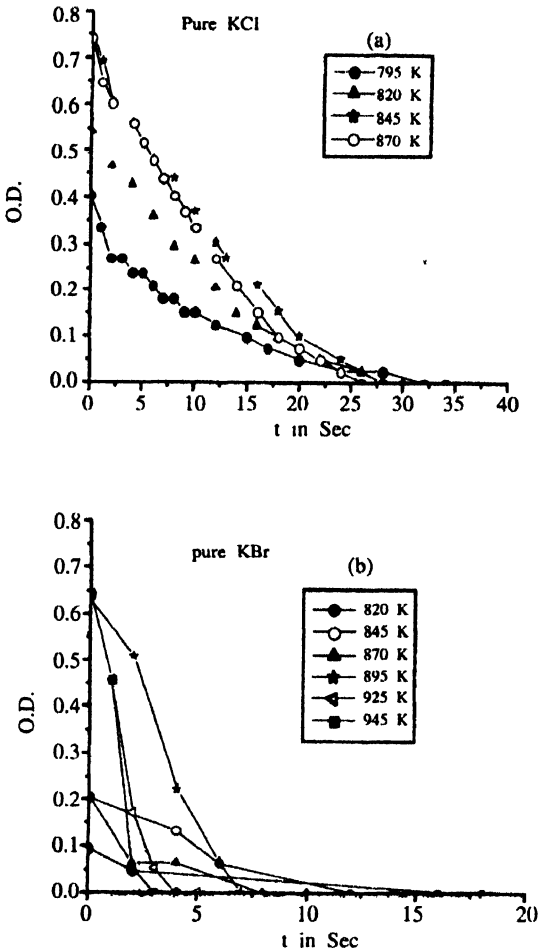


Figure 3. Change of optical density (OD) during decay process at different temperature for (a) pure KCl and (b) pure KBr.

From transition point as the crystal attains its original transparency, the time of blecaching has been found out and mobility (μ) has been calculated from the eq. [8]

$$\mu = L^2/tV,$$

where L is the effective length of the crystal, V is the applied potential in Volt and t is the transition time. The dependence of transition time on temperature [$t = f(T)$] leads to find a relation like

$$\mu = \mu_0 \exp(-W_F/kT),$$

where, W_F is the activation energy of bleaching, k is the Boltzmann constant and T is the temeprature in absolute scale.

If we plot $\left[\ln(\mu) \sim \frac{1}{T}\right]$ (Figure 4), it gives straight line and the slope of the straight line gives the activation energy for bleaching or migration of F-center by injected electrons.

Again we know, $W_F = E_F - W/2$,

where E_F is the energy required to dissociate the F-center thermally and W is the energy required to form a

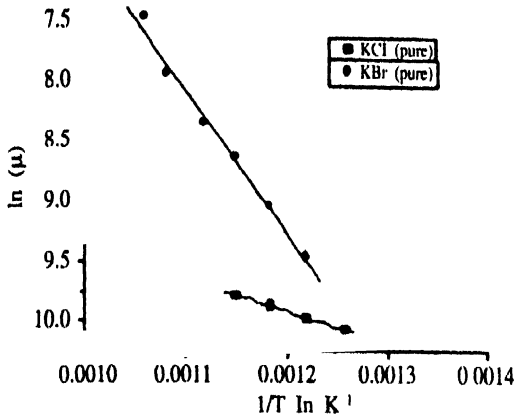


Figure 4. Plot of $\ln(\mu)$ against $1/T$ in K^{-1}.

Schottky defect. From the experimentally determined values of W_F we can have an idea of E_F (Table 1).

Table 1. Activation energy (W_F) and dissociation energy (E_f) for mobility of different specimens.

Specimen	Activation energy (W_f) in eV	Dissociation energy (E_f) in eV
KCl (pure)	0.224	1.224
KBr (pure)	1.007	2.007

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